β-HgO_2 Structure: AB2_oP12_61_a_c-001

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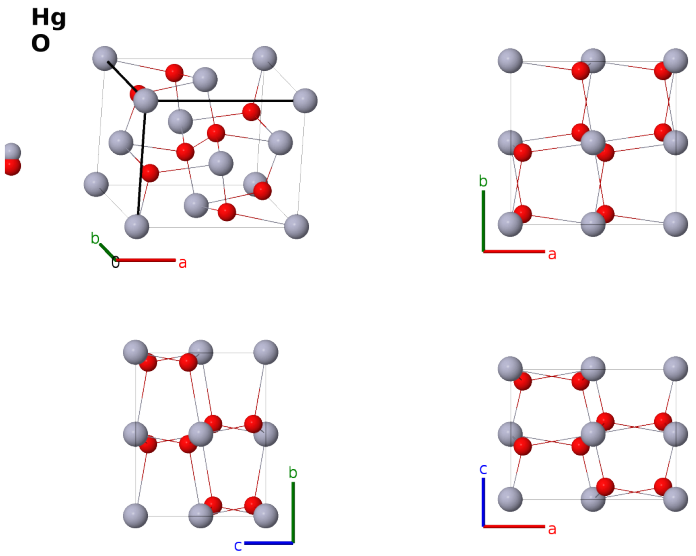
https://aflow.org/prototype-encyclopedia/JQ93

https://aflow.org/prototype-encyclopedia/AB2_oP12_61_a_c-001

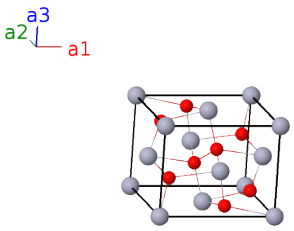


Prototype	HgO_2
AFLOW prototype label	AB2_oP12_61_a_c-001
ICSD	24774
CCDC	1600786
Pearson symbol	oP12
Space group number	61
Space group symbol	*Pbca*
AFLOW prototype command	`aflow --proto=AB2_oP12_61_a_c-001 --params=`$a, b/a, c/a, x_2, y_2, z_2$

- HgO_2 exists as
  - monoclinic α-HgO and
  - orthorhombic β-HgO_2 (this structure).
- β-HgO_2, AgF_2, and $PdSe_2$ have the same AFLOW prototype label, AB2_oP12_61_a_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Hg I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Hg I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Hg I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4a)	Hg I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_{11}}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	O I

References

[1] N. G. Vannerberg, *Formation and structure of mercuric peroxides*, Arkiv für Kemi **13**, 515–521 (1959).

First cited in

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